Journal of Applied Physics 2013 vol.114 N16

Parametric hierarchical matrix approach for the wideband optical response of large-scale molecular aggregates

Ansari-Oghol-Beig D., Rostami M., Chernobrovkina E., Saikin S., Valleau S., Mosallaei H., Aspuru-Guzik A.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

Fast and efficient calculations of optical responses using electromagnetic models require computational acceleration and compression techniques. A hierarchical matrix approach is adopted for this purpose. In order to model large-scale molecular structures, these methods should be applied over wide frequency spectra. Here, we introduce a novel parametric hierarchical matrix method that allows one for a rapid construction of a wideband system representation and enables an efficient wideband solution. We apply the developed method to the modeling of the optical response of bacteriochlorophyll tubular aggregates as found in green photosynthetic bacteria. We show that the parametric method can provide one with the frequency and time-domain solutions for structures of the size of 100 000 molecules, which is comparable to the size of the whole antenna complex in a bacterium. The absorption spectrum is calculated and the significance of electrodynamic retardation effects for relatively large structures, i.e., with respect to the wavelength of light, is briefly studied.

http://dx.doi.org/10.1063/1.4826189